these challenges. Our thesis is that crystal growth modeling is a powerful tool to complement experiments and characterization. It provides an important approach to close the loop between materials discovery, device research, systems performance, and producibility

Specifically, we discuss our efforts to model gradient freeze furnaces used to grow large CZT crystals at Pacific Northwest National Laboratories and Washington State University. Model results are compared with experimental measurements, and the insight gained from modeling is discussed. Of particular interest is how different growth strategies are predicted to impact the shape of the crystal interface. We also address ongoing research, including the development of models for realistic, three-dimensional computations, meso-scale models for second-phase particle formation and movement, and model-based controllers for crystal growth.

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R05-4: Growth, Nanostructures, and Heat Treatment of High Resistivity Cd1-xZnxTe Crystals

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Cd1-xZnxTe (CZT) crystal possesses excellent optoelectronic properties and is therefore one of the most promising materials for room temperature X-ray and gamma-ray detectors. Although the study on CZT has lasted for a long period, there still exist some problems in the preparation, characterization and upgradation of CZT, which are explored in this work. A modified vertical Bridgman method (VBM) has been proposed and succeeded in growing CZT ingots with the dimensions up to $\Phi 60\times 150$ mm^2. Investigations indicate that the modified VBM is very efficient to reduce the defects density and consequently upgrade optoelectronic properties of CZT crystals. High resolution electron microscopy (HREM) has revealed the atomic structures of defects including dislocations, Te precipitates, and twins in CZT, based on which their formation mechanism has been discussed in depth. Study of the influence of various impurities on the structural and optoelectronic properties of CZT has guided us to choose the appropriate dopants for CZT. Finally, several annealing procedures are adopted to further improve the CZT properties.

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R05-5: Dewetting During Crystal Growth of (Cd,Zn)Te:In under Microgravity

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The phenomenon of “Dewetting” during crystal growth has been observed in several microgravity experiments for different semiconductor crystals. The results of these experiments showed an improvement of the material quality due to the contact-less growth of the crystals. A number of crystal growth techniques have been used to grow CZT. The most widely used is the growth from the melt by the Bridgman method. However the crucible, which is generally made of carbon-layered silica glass, causes a number of problems: solid-liquid interface curvature, spurious nucleation of grains and twins, thermal stresses during the cooling of the crystal. This work is concentrated on the growth of high resistivity (Cd,Zn)Te:In (CZT) crystals by using the phenomenon of dewetting and its application in the processing of CZT detectors. Two Cd0.9Zn0.1Te:In crystals were grown under microgravity on the Russian FOTON satellite in the Polizon facility in September 2007. One crystal was grown under a rotating magnetic field during the phase of homogenization to destroy the typical tellurium clusters in the melt. The other crystal was superheated with 20 K above the melting point. A third crystal has been grown on the ground in similar thermal conditions. Inspection of the surface of the space grown crystals gave the evidence of successful dewetting during the crystal growth. The influence of the dewetting on the material properties is shown by the results of optical and electrical characterization methods. Finally, CZT detectors have been processed from the grown part of the different crystals. The influence of dewetting on their performance will be studied by means of the detector measurements with X- and Gamma-ray sources.